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Re: Annual Report for N00014-90-J-1267

To whom it may concern:

Enclosed is the Annual Report for N00014-90-J-1267. The report was prepared by Principal Investigator, Professor Y.-C. Chang.

If you require additional information, please let me know.

Sincerely,

Carolyn J. Wright

Carolyn J. Wright
Program Administrative Assistant

CW
encs.
cc/enc: Y. C. Chang
Grants & Contracts, UIUC

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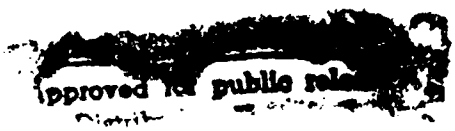

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ANNUAL REPORT (Oct.1, 1992 - Sept. 30, 1993)

CONTRACT NO.: ONR N00014-90-J-1267

PRINCIPAL INVESTIGATOR: Yia-Chung Chang

RESEARCH ASSOCIATES: S.-F. Ren/ Z.-Q. Gu

I. OBJECTIVE:

To understand the electronic structures of semiconductor surfaces and heterostructures in relation to crystal growth.

II. APPROACH:

Perform first-principle theoretical calculations to determine the structures of surface and interface identify the main spectral features of the reflectance-difference spectra of (001) GaAs with transitions involving Ga-Ga dimers and As-As dimers.

III. PROGRESS:

A. Electronic Properties of $(ZnSe)_m(Cd_{1-x}Zn_xSe)_n$ Supe lattices

We performed theoretical calculations on the electronic structures of $(ZnSe)_m(Cd_{1-x}Zn_xSe)_n$ superlattices. First-principle pseudopotential calculations are used to obtain the valence-band offset for CdSe grown on ZnSe. We then use an empirical non-local pseudopotential method to calculate the band structures and effective masses of $(ZnSe)_m(Cd_{1-x}Zn_xSe)_n$ superlattices grown on ZnSe, including the spin-orbit interaction. The effects of strain due to lattice mismatch have been properly taken into account. We have also studied the band gap as a function of composition and layer thicknesses of constituent materials in superlattices. The results are in agreement with recent experiment. The quantum well made from these materials is an important candidate for quantum-well lasers operating in the blue-green wavelengths.

B. Calculation of surface structures with large reconstructions

We have recently developed a first-principle pseudopotential method based on a new planar-like basis. We have successfully applied the new method to study the electronic structures and work function of Si (001) 2×1 surface with symmetric dimer reconstruction with and without hydrogen passivation. We have calculated the work function of the Si

(001) 2×1 surface with hydrogen passivation. We have also calculated the hydrogen dissociation energy and the result is in accord with previous experimental findings.[14,15]

Furthermore, we have constructed the "planar Wannier orbitals" by using linear combinations of these orbitals at the zone center and zone boundary for each in-p'ane wave vector, $k_{||}$. Only eight planar Wannier orbitals per atomic layer are needed to reproduce the bulk band structure accurately throughout the entire Brillouin zone. With the $k_{||}$-dependent interaction parameters between planar Wannier orbitals calculated and stored, we essentially convert a first-principle calculation into a simple tight-binding calculation. Another advantage of using planar Wannier orbitals is that the surface Green's function can evaluated accurately and efficiently using the complex-band structure method. Equipped with this tool, we are now ready to attack surfaces with more complicated reconstructions, such as the GaAs (001) 2×4 surface.

Publications supported by ONR-N00014-90-J-1267
(Oct. 1, 1992 – Sept. 30, 1993)

1. **Optical study of $(Al_xGa_{1-x})_{0.5}In_{0.5}P/GaAs$ Semiconductor Alloys by Spectroscopic Ellipsometry**, H. Lee, M. V. Klein, D. E. Aspnes, C. P. Kuo, M. Peanasky, and M. G. Craford, J. Appl. Phys. **73**, 400 (1993).

Papers submitted to refereed journals:

1. **Electronic Properties of $ZnSe_m(Cd_{1-x}Zn_xSe)_n$ superlattices**, S. F. Ren, Z. Gu, and Y. C. Chang, Phys. Rev. B (in press).

2. **Optical Properties of the Zincblende CdSe and $Zn_xCd_{1-x}Se$ films grown on GaAs** Y. D. Kim, M. V. Klein, S. F. Ren, Y. C. Chang, H. Luo, N. Samarth, and J. K. Furdyna, Phys. Rev. B (in press).

3. **Electronic Structures and Optical Properties of $[ZnSe_m(CdSe)_n]_N$-ZnSe Multi-quantum Wels**, S. F. Ren, J. B. Xia, H. X. Han, and Y. C. Chang, J. Appl. Phys. (submitted).